



PTO/SB/21 (03-03)

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**TRANSMITTAL  
FORM**

(to be used for all correspondence after initial filing)

<b>TRANSMITTAL FORM</b>  (to be used for all correspondence after initial filing)	Application Number	10/053,348	
	Filing Date	November 2, 2001	
	First Named Inventor	Rosenthal, Dan E.	
	Art Unit	2123	
	Examiner Name	Unassigned	
Total Number of Pages in This Submission	7	Attorney Docket Number	020910-000310US

**ENCLOSURES (check all that apply)**

- ☐ Fee Transmittal Form
- ☐ Fee Attached
- ☐ Amendment / Reply
  - ☐ After Final
  - ☐ Affidavits/declaration(s)
- ☐ Extension of Time Request
- ☐ Express Abandonment Request
- ☒ Information Disclosure Statement
- ☐ Certified Copy of Priority Document(s)
- ☐ Response to Missing Parts/  
Incomplete Application
  - ☐ Response to Missing  
Parts under 37 CFR  
1.52 or 1.53

- ☐ Assignment Papers
- ☐ Drawing(s)
- ☐ Licensing-related Papers
- ☐ Petition Routing Slip (PTO/SB/69)  
and Accompanying Petition
- ☐ Petition to Convert to a  
Provisional Application
- ☐ Power of Attorney, Revocation  
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- ☐ After Allowance Communication to  
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- ☐ Proprietary Information
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Remarks

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**SIGNATURE OF APPLICANT, ATTORNEY, OR AGENT**

Firm or Individual	Protein Mechanics, Inc. Charles K. Sholtz	Reg. No. 38,615
Signature		
Date	March 21, 2003	

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Attorney Docket No.: 020910-000310US <sup>PATENT</sup>

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re application of:

Dan E. Rosenthal

Application No.: 10/053,348

Filed: November 2, 2001

For: METHOD FOR ANALYTICAL  
JACOBIAN COMPUTATION IN  
MOLECULAR MODELING

Examiner: Unassigned

Art Unit: 2123

SUPPLEMENTAL INFORMATION  
DISCLOSURE STATEMENT UNDER 37  
CFR §1.97 and §1.98

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Assistant Commissioner for Patents  
Washington, D.C. 20231

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Sir:

The references cited on attached form PTO/SB/08A and PTO/SB/08B are being called to the attention of the Examiner. Copies of the references are enclosed. It is respectfully requested that the cited references be expressly considered during the prosecution of this application, and the references be made of record therein and appear among the "references cited" on any patent to issue therefrom.

As provided for by 37 CFR 1.97(g) and (h), no representation is being made that a search has been conducted or that this statement encompasses all the possible relevant information, and no inference should be made that the information and references cited are, or are considered to be material to patentability because they are in this statement. No inference should be made that the information and references cited are prior art merely because they are in this statement.

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However, if a fee is required, the Commissioner is authorized to deduct such fee from the undersigned's Deposit Account No. 50-2599. Please deduct any additional fees from, or credit any overpayment to, the above-noted Deposit Account.

Respectfully submitted,

A handwritten signature in dark ink, appearing to be 'CS' followed by a long horizontal stroke.

Charles K. Sholtz  
Reg. No. 38,615

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**INFORMATION DISCLOSURE  
STATEMENT BY APPLICANT**

(use as many sheets as necessary)

Sheet 1 of 3**Complete if Known**

Application Number	10/053,348
Filing Date	November 2, 2001
First Named Inventor	Rosenthal, Dan E.
Art Unit	2123
Examiner Name	Unassigned
Attorney Docket Number	020910-000310US

**U.S. PATENT DOCUMENTS**

Examiner	Cite No. <sup>1</sup>	Document Number	Publication Date MM-DD-YYYY	Name of Patentee or Applicant of Cited Document	Pages, Columns, Lines, Where Relevant Passages or Relevant Figures Appear
		Number Kind Code <sup>2</sup> (if known)			
	AA	US 6,512,997	1/28/2003	Padilla, et al.	
	AB	US 6,185,506	2/6/2001	Cramer, III, et al.	
	AC	US 6,161,080	12/12/2000	Aouni-Ateshian, et al.	
	AD	US 6,125,235	9/26/2000	Padilla, et al.	
	AE	US 6,081,766	6/27/2000	Chapman, et al.	
	AF	US 6,014,449	1/11/2000	Jacobs, et al.	
	AG	US 5,787,279	7/28/1998	Rigoutsos	
	AH	US 5,777,889	7/7/1998	Mohanty, et al.	
	AI	US 5,752,019	5/12/1998	Rigoutsos, et al.	
	AJ	US 5,745,385	4/28/1998	Hinsberg, III, et al.	
	AK	US 5,625,575	4/29/1997	Goyal, et al.	
	AL	US 5,553,004	9/3/1996	Gronbech-Jensen, et al.	
	AM	US 5,307,287	4/26/1994	Cramer, III, et al.	

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**FOREIGN PATENT DOCUMENTS**

Examiner Initials*	Cite No. <sup>1</sup>	Foreign Patent Document			Publication Date MM-DD-YYYY	Name of Patentee or Applicant of Cited Document	Pages, Columns, Lines, Where Relevant Passages or Relevant Figures Appear	T <sup>2</sup>
		Country Code <sup>3</sup>	Number <sup>4</sup>	Kind Code <sup>5</sup> (if known)				
	AN	WO	02/073334	A2	07-26-1990	Padilla, et al.		<input type="checkbox"/>
	AO	WO	01/67310	A1	12-12-1991	Smith, et al.		<input type="checkbox"/>
	AP	WO	96/24902	A1	04-01-1993	Wertz		<input type="checkbox"/>

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**OTHER PRIOR ART -- NON PATENT LITERATURE DOCUMENTS**

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✓	AQ	ASCHER, et al., <u>Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations</u> , 1998, pgs. 3-122 and 231-297, SIAM, Philadelphia, PA.	
✓	AR	BARAFF, et al., " <u>Large steps in cloth simulation</u> ", 1998, <u>Computer Graphics Proceedings SIGGRAPH 98</u> (Orlando, July 19-24) p43.pdf	
	AS	BARTH, et al., " <u>A separating framework for increasing the timestep in molecular dynamics</u> " in <u>Computer Simulation of Biomolecular Systems - Theoretical and Experimental Applications, Volume 3</u> , 1997, pgs. 97-121, Kluwer AcademicDordrecht, The Netherlands.	

Examiner Signature	Date Considered
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# INFORMATION DISCLOSURE STATEMENT BY APPLICANT

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Sheet 2 of 3

## Complete if Known

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✓	AT	BERENDSEN, "Molecular Dynamics Simulations: The Limits and Beyond" in <u>Computational Molecular Dynamics: Challenges, Methods, Ideas</u> , 1999, pgs. 3-36, Springer-Verlag, Germany.	
✓	AU	BISCHOF, et al., <u>ADIFOR 2.0 Users' Guide</u> , 1998, Argonne National Laboratory, University of Chicago, Argonne, IL.	
✓	AV	BRENAN, et al., <u>Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations</u> , 1989, Chapter 5 (pgs. 115-148), Elsevier Science Publishing Co., New York, NY.	
✓	AW	BUTCHER, "Towards efficient implementation of singly-implicit methods", 1988, <u>AMC Transactions of Mathematical Software</u> 14:68-75.	
✓	AX	BYSTROFF, "An alternative derivation of the equations of motion in torsion space for a branched linear chain", 2001, <u>Protein Engineering</u> 14:825-828.	
✓	AY	COLEMAN, et al., "The efficient computation of sparse Jacobian matrices using automatic differentiation", 1996, <u>Cornell Theory Center Technical Report</u> CTC95TR225.	
	AZ	EICHBERGER, et al., "The benefits of parallel multibody simulation", 1994, <u>International Journal for Numerical Methods in Engineering</u> , 37:1557-1572.	
✓	BA	GOLUB, et al., "The Differentiation of Pseudo-Inverses and Non-Linear Least Squares Problems Whose Variables Separate", 1973, <u>SIAM J. Numer. Anal.</u> 10:413.	
✓	BB	HAIRER, et al., <u>Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems</u> , 2nd ed., 1996, Springer-Verlag, Germany.	
✓	BC	HE, et al., "Macromolecular conformational dynamics in torsional angle space", 1998, <u>Journal of Chemical Physics</u> 108:271.	
✓	BD	HOLLARS, et al., <u>SD/FAST User's Manual, Version B.2</u> , 1994, Symbolic Dynamics, California.	
✓	BE	IZAGUIRRE, et al., "Longer Time Steps for Molecular Dynamics", 1999, <u>J.Chem.Phys.</u> 110:9853.	
	BF	KANE, <u>Dynamics</u> , 3rd ed., 1978, Stanford University, Stanford, California.	
	BG	LEACH, <u>Molecular Modelling Principles and Applications</u> , 2nd ed., 1996, Chapter 6 (pgs. 303-352) Pearson Education Limited, England.	

Examiner Signature		Date Considered	
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✓	BH	MARTINS, et al., "An automated method for sensitivity analysis using complex variables", 2000, <u>American Institute of Aeronautics and Astronautics</u> , 2000-0689 p1	
✓	BI	NORSETT, et al., "Embedded SDIRK-methods of basic order three", 1984, <u>BIT</u> 24:634-646.	
✓	BJ	PONDER, <u>TINKER User's Guide, Version 3.8</u> , October 2000, Washington University, St. Louis, MO.	
✓	BK	RAPAPORT, <u>The Art of Molecular Dynamics Simulation</u> , 1995, reprinted with corrections 1998, Chapter 3 (pgs. 42-77), Cambridge University Press, United Kingdom.	
✓	BL	SCHLICK, "Biomolecular Dynamics at Long Timesteps: Bridging the Timescale Gap Between Simulation and Experimentation", 1997, <u>Annu. Rev. Biophys. Biomol. Struct.</u> , 26:181-222.	
✓	BM	SCHLICK, "Some Failures and Successes of Long-Timestep Approaches to Biomolecular Simulations" in <u>Computational Molecular Dynamics: Challenges, Methods, Ideas</u> , 1999, pgs. 227-262, Springer-Verlag, Germany.	
	BN ✓	SCHLICK, <u>Molecular Modeling and Simulation - An Interdisciplinary Guide</u> , 2002, Chapter 13 and References, pgs. 419-462 and 561-619, Springer-Verlag, Germany.	
	BO ✓	SHAMPINE, "Implementation of implicit formulas for the solution of ODEs", 1980, <u>SIAM J. Sci. Stat. Comput.</u> 1:103-118.	
✓	BP	VERLET, "Computer Experiments on Classical Fluids. I. Thermodynamical Properties of Lennard-Jones Molecules", 1967, <u>Physical Review</u> , 159(1):98-103.	
✓	BQ	VON SCHWERIN, <u>Multibody System Simulation</u> , 1999, Springer-Verlag, Germany.	
✓	BR	WU, et al., "Constraint dynamics algorithm for simulation of semiflexible macromolecules", 1998, <u>Journal of Computational Chemistry</u> 19:1555-1566	
✓	BS	YEN, et al., "On the numerical solution of constrained multibody dynamic systems", 1994, <u>University of Minnesota AHPARC</u> 94-038.	

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